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(71) Applicant (for all designated States except US): **3-DI-MENSIONAL PHARMACEUTICALS, INC.** [US/US];  
Three Lower Makefield Corporate Center, 1020 Stony Hill  
Road, Suite 300, Yardley, PA 19067 (US).

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(72) Inventors; and

(75) Inventors/Applicants (for US only): **AGRAFIOTIS, Dimitris, K.** [US/US]; 660 Perimeter Drive, Downingtown, PA 19335 (US). **XU, Huafeng** [CN/US]; 128 Kirkham Street, San Francisco, CA 94122 (US). **IZRAILEV, Sergei, F.** [RU/US]; 125 Christopher Street, Apartment 3B, New York, NY 10014 (US). **SALEMME, Francis, R.** [US/US]; 1970 Timber Lakes Drive, Yardley, PA 19067 (US).

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(74) Agents: **NORTON, Vicky, G.** et al.; Pillsbury Winthrop, LLP, 11682 El Camino Real, Suite 200, San Diego, CA 92130-2593 (US).

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(54) Title: CONFORMATIONAL SAMPLING BY SELF-ORGANIZATION

(57) Abstract: A self-organizing method, system, and computer program product for generating molecular conformations that are consistent with a set of distance and/or volume constraints. A stochastic proximity embedding (SPE) algorithm evaluates individual distance and/or volume constraints and adjusts the atomic coordinates to minimize violations of such constraints. The method scales linearly with the number of atoms, and produces many more unique conformations at a fraction of the time required by conventional distance geometry algorithms.

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## INTERNATIONAL SEARCH REPORT

International application No.

PCT/US03/19905

## A. CLASSIFICATION OF SUBJECT MATTER

IPC(7) : G01N 33/48

US CL : 702/19

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 702/19

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)  
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## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
Y	FEUSTON et al. Comparison of Knowledge-based and Distance Geometry. Approaches for Generation of Molecular Conformation. J. Chem. Inf. Comput. Sci. 2001, Vol. 41, pages 754-763. Entire document.	1-12
Y	HUANG et al. Distance Geometry Generates Native-like Folds for Small Helical Proteins Using the Consensus Distances of Predicted Protein Structures. Protein Science. 1998, Vol. 7, pages 1998-2003. Entire document.	1-12
A	US 6,269,312 B1 (MAYO et al) 31 July 2001 (31.07.2001) especially columns 5-72.	1-12
A	US 5,241,470 A (LEE et al) 31 August 1993 (31.08.1993), especially columns 4-27.	1-12
A	US 5,553,004 A (GRONBECH-JENSEN et al) 03 September 1996 (03.09.1996), especially columns 6-26.	1-12
A	US 6,150,179 A (WENT) 21 NOVEMBER 2000 (21.11.2000), especially columns 5-61.	1-12



Further documents are listed in the continuation of Box C.



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Name and mailing address of the ISA/US

Mail Stop PCT, Attn: ISA/US  
Commissioner for Patents  
P.O. Box 1450  
Alexandria, Virginia 22313-1450

Facsimile No. (703)305-3230

Authorized officer

Shubo "Joe" Zhou

Telephone No. (703)-308-0196

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**Continuation of B. FIELDS SEARCHED Item 3:**  
EAST and STN